

Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric Result

logP (XH +) 0.87 ±0.03 (n=50)
 logP (neutral X) 3.95 ±0.01 (n=50)
 RMSD 0.342

18C-24003 Points 1 to 26

M04_octanol concentration factor 0.985
 Carbonate 0.1126 mM
 Acidity error 0.07154 mM

18C-24003 Points 27 to 52

M04_octanol concentration factor 0.875
 Carbonate 0.1064 mM
 Acidity error -0.19519 mM

18C-24003 Points 53 to 77

M04_octanol concentration factor 0.960
 Carbonate 0.1188 mM
 Acidity error 0.08198 mM

Warnings and errors

Errors None
 Warnings None

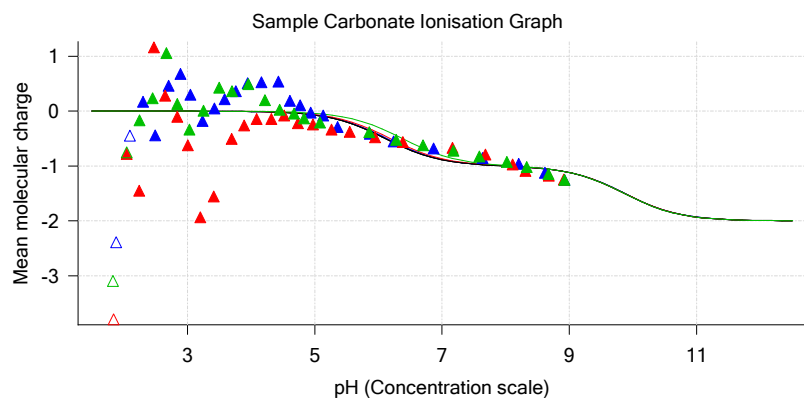
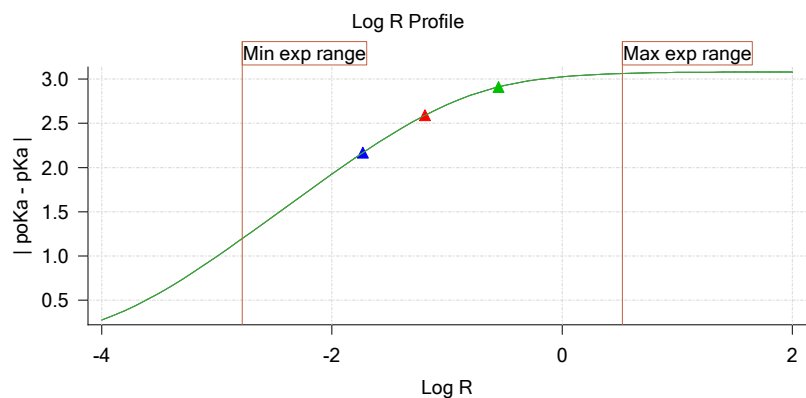
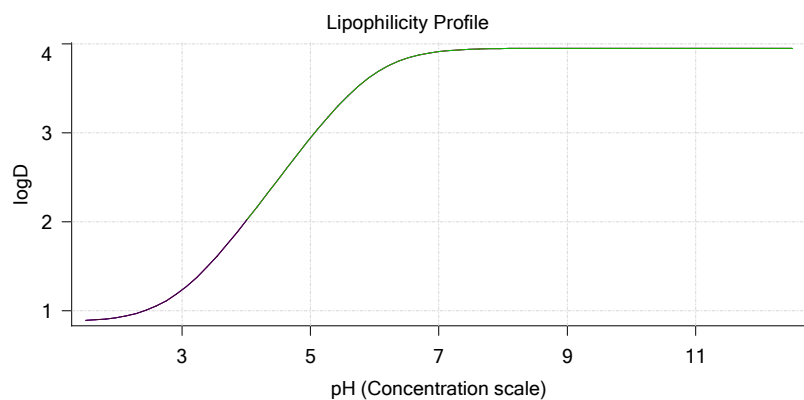
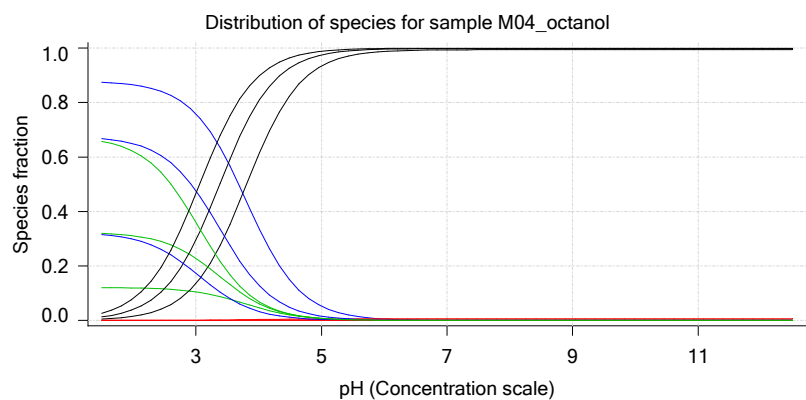
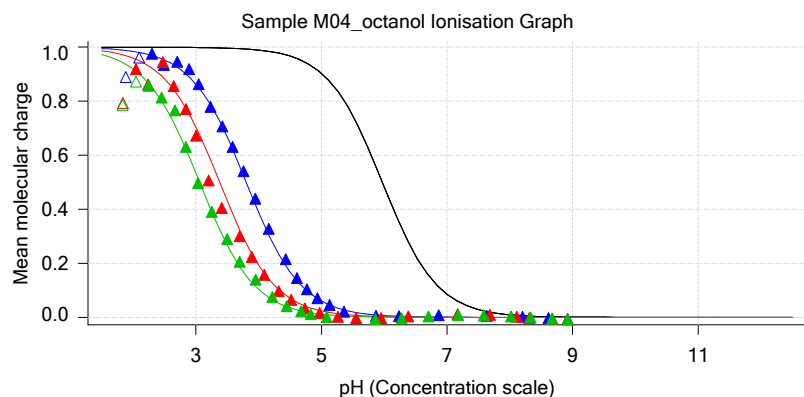
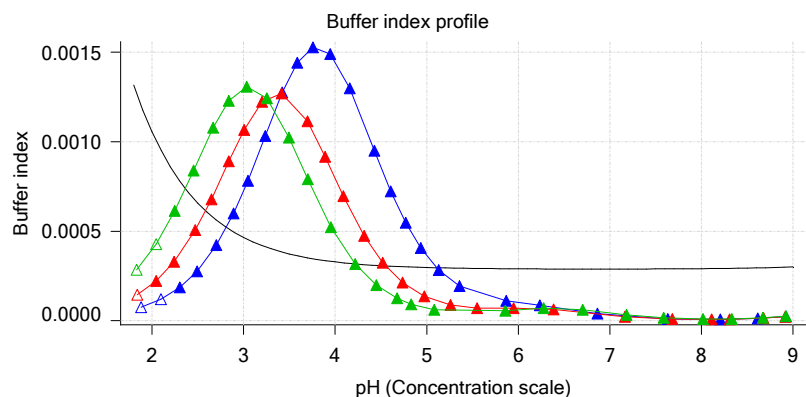
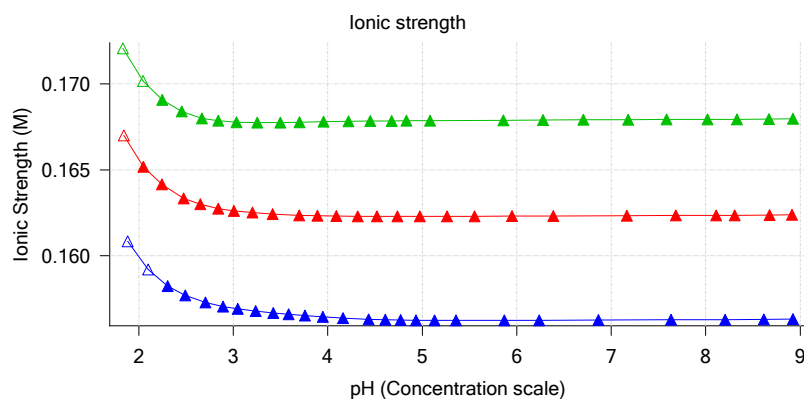
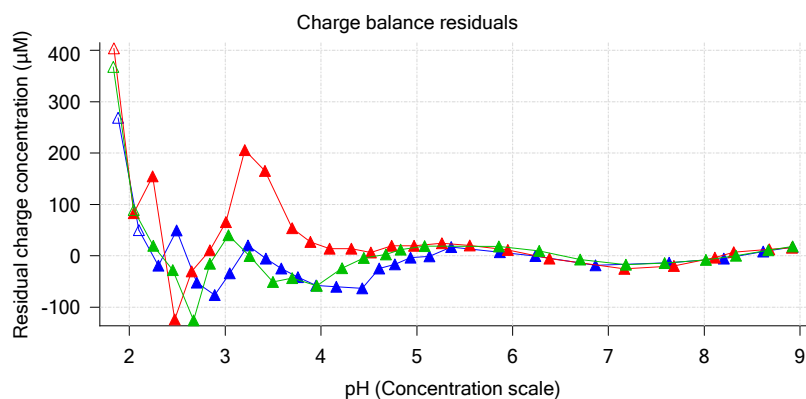
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.88	11.71 %	0.00 %	87.17 %	1.12 %	Stomach pH
1.200	0.88	11.63 %	0.00 %	86.60 %	1.77 %	
2.000	0.92	10.63 %	0.00 %	79.16 %	10.20 %	
3.000	1.23	5.54 %	0.01 %	41.26 %	53.19 %	
4.000	2.01	0.96 %	0.01 %	7.13 %	91.90 %	Blood pH
5.000	2.94	0.10 %	0.01 %	0.77 %	99.12 %	
6.000	3.67	0.01 %	0.01 %	0.08 %	99.90 %	
6.500	3.84	0.00 %	0.01 %	0.02 %	99.96 %	
7.000	3.91	0.00 %	0.01 %	0.01 %	99.98 %	
7.400	3.94	0.00 %	0.01 %	0.00 %	99.99 %	
8.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	

Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

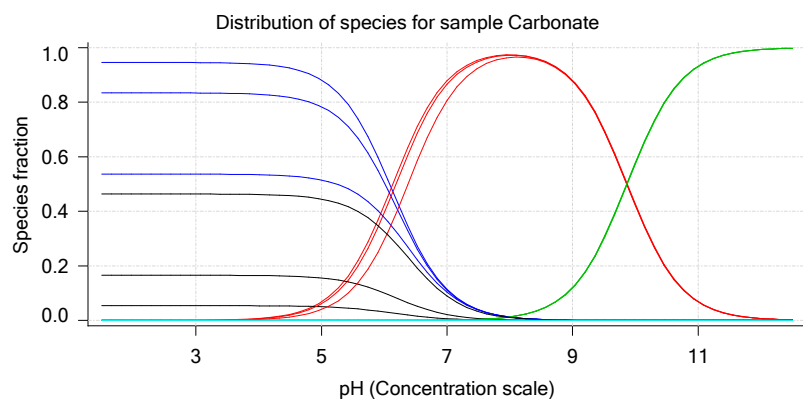
Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T312060**

Graphs



Sample name:	M04_octanol	Experiment start time:	3/24/2018 2:50:31 AM
Assay name:	pH-metric high logP	Analyst:	Dorothy Levorse
Assay ID:	18C-24003	Instrument ID:	T312060
Filename:	C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r		

Graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-24003 Points 1 to 26

Overall results

RMSD 0.279
 Average ionic strength 0.157 M
 Average temperature 24.9°C
 Partition ratio 0.0186 : 1
 Analyte concentration range 2638.8 µM to 2719.9 µM
 Total points considered 24 of 26

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Parameter	Value	Date/Time	File
Alpha	0.119	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
S	0.9972	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
jH	0.9	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
jOH	-0.3	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r

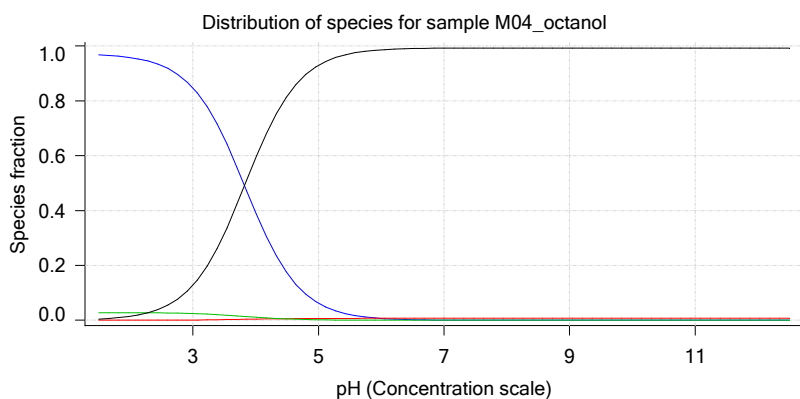
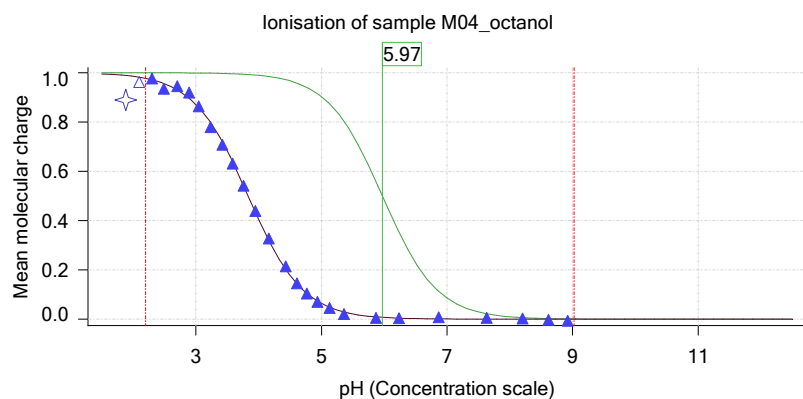
Titants

Concentration	Value	Date/Time	File
0.50 M HCl	0.997124	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
0.50 M KOH	1.003190	3/24/2018 2:50:31 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

M04_octanol concentration factor	0.985
Base pKa 1	5.97
logP (XH +)	0.19
logP (neutral X)	3.88

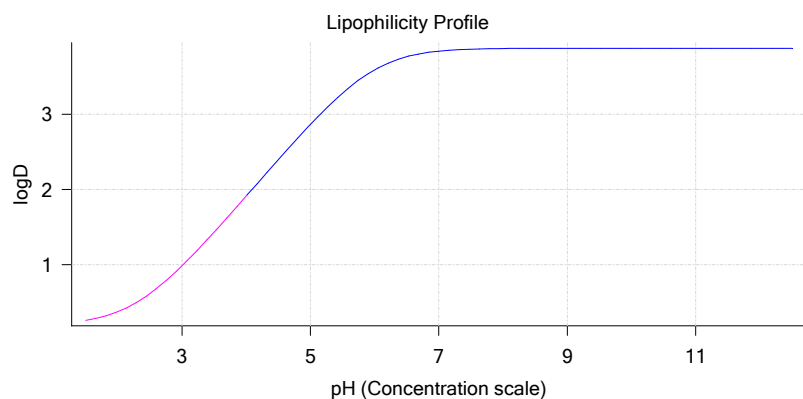
Sample graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**



Sample graphs (continued)



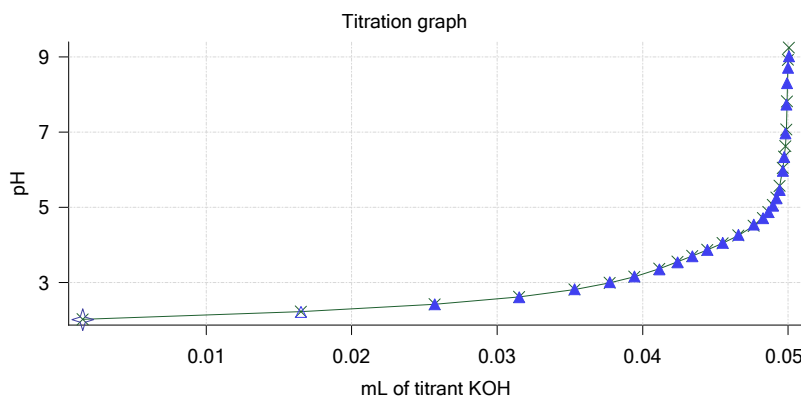
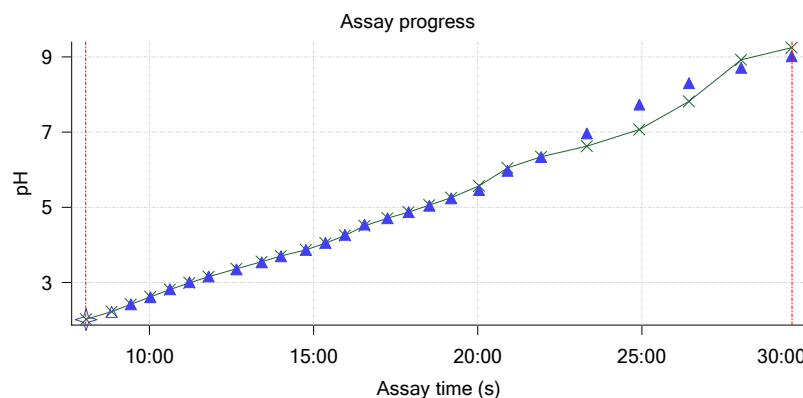
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanolH	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.21	97.06 %	0.00 %	2.79 %	0.15 %	Stomach pH
1.200	0.22	96.98 %	0.00 %	2.79 %	0.23 %	
2.000	0.37	95.80 %	0.01 %	2.75 %	1.44 %	
3.000	0.98	84.73 %	0.09 %	2.44 %	12.75 %	
4.000	1.91	39.31 %	0.42 %	1.13 %	59.14 %	
5.000	2.87	6.18 %	0.66 %	0.18 %	92.98 %	Blood pH
6.000	3.59	0.66 %	0.70 %	0.02 %	98.62 %	
6.500	3.77	0.21 %	0.71 %	0.01 %	99.08 %	
7.000	3.84	0.07 %	0.71 %	0.00 %	99.23 %	
7.400	3.86	0.03 %	0.71 %	0.00 %	99.27 %	
8.000	3.87	0.01 %	0.71 %	0.00 %	99.29 %	
9.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	
10.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	
11.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	
12.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	

Carbonate and acidity

 Carbonate 0.113 mM
 Acidity error 0.072 mM

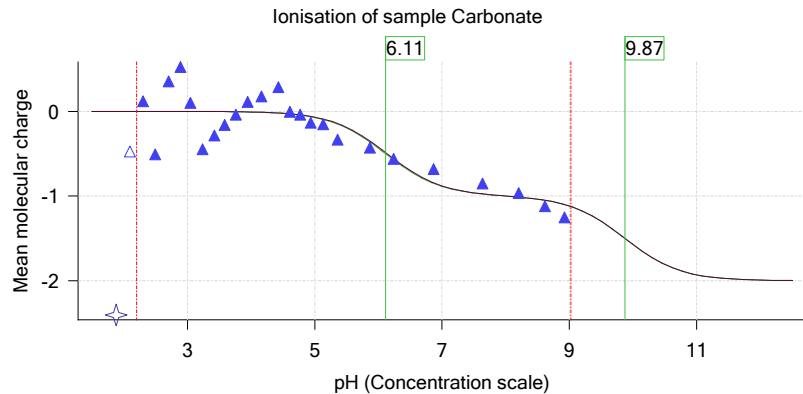
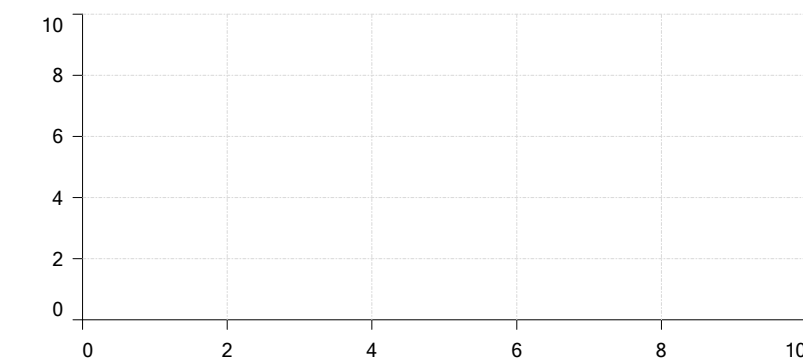
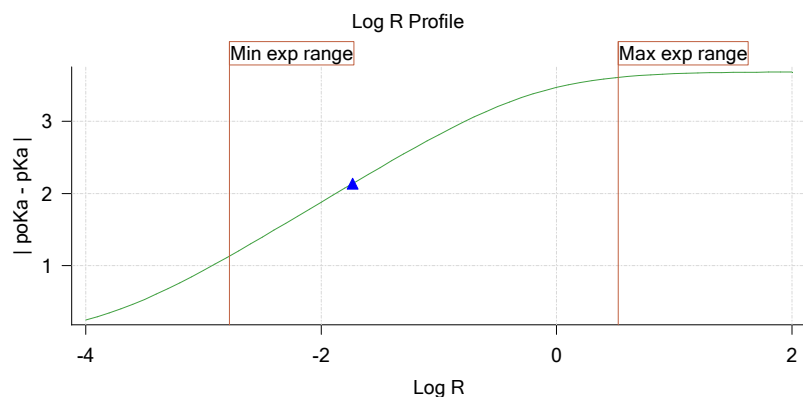
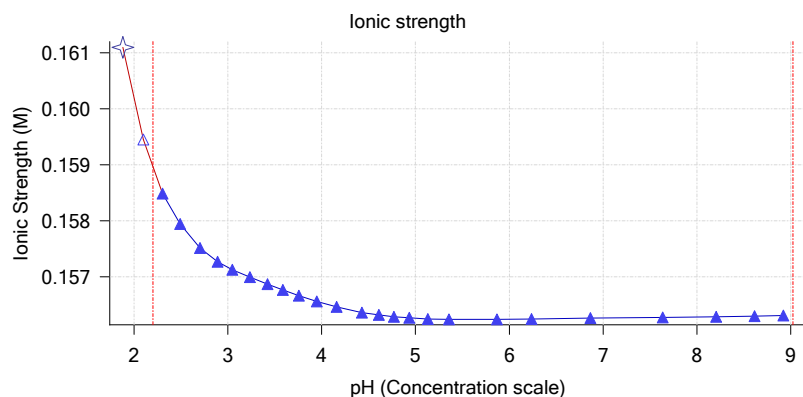
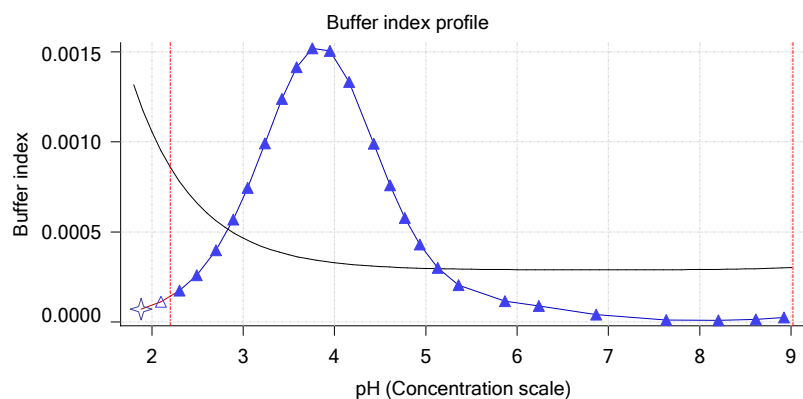
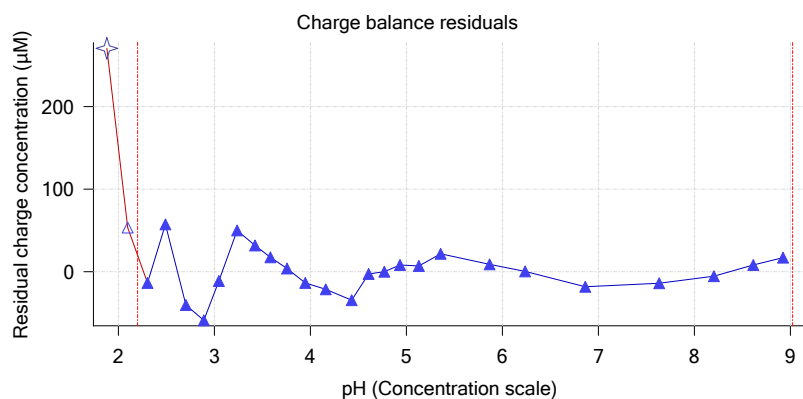
Other graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-24003 Points 27 to 52





Overall results

RMSD 0.447
 Average ionic strength 0.163 M
 Average temperature 25.0°C
 Partition ratio 0.0643 : 1
 Analyte concentration range 2363.9 µM to 2436.4 µM
 Total points considered 25 of 26



Warnings and errors

Errors None
 Warnings None





Four-Plus parameters

	Alpha	0.119	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
	S	0.9972	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
	jH	0.9	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
	jOH	-0.3	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r

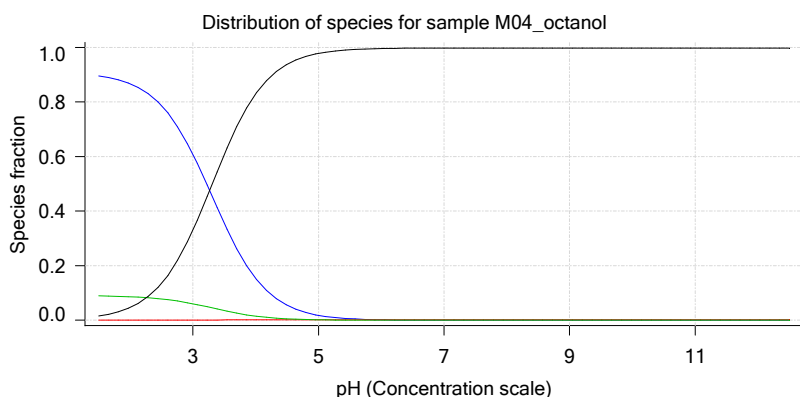
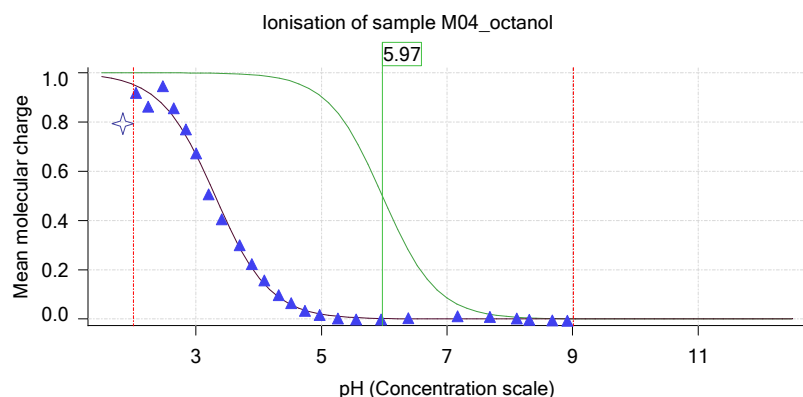
Titrants

	0.50 M HCl	0.997124	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
	0.50 M KOH	1.003190	3/24/2018 2:50:31 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

	M04_octanol concentration factor	0.875
	Base pKa 1	5.97
	logP (XH +)	0.19
	logP (neutral X)	3.90

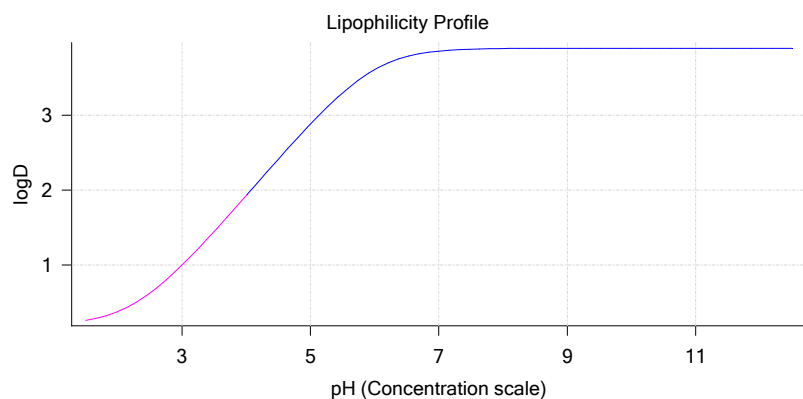
Sample graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T312060**

Sample graphs (continued)



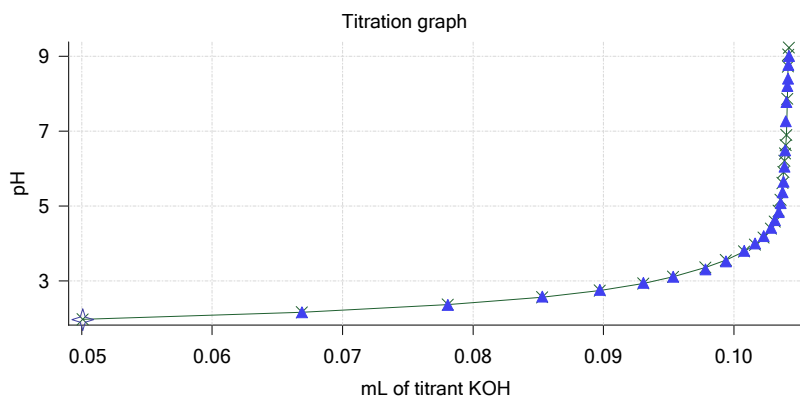
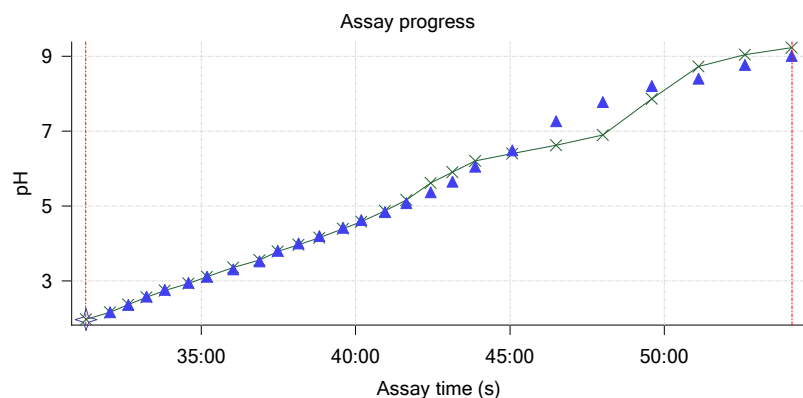
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.21	90.50 %	0.00 %	9.01 %	0.49 %	Stomach pH
1.200	0.23	90.24 %	0.00 %	8.99 %	0.77 %	
2.000	0.38	86.67 %	0.01 %	8.63 %	4.69 %	
3.000	1.00	60.90 %	0.07 %	6.07 %	32.97 %	
4.000	1.93	15.33 %	0.16 %	1.53 %	82.98 %	
5.000	2.88	1.81 %	0.19 %	0.18 %	97.82 %	Blood pH
6.000	3.61	0.18 %	0.20 %	0.02 %	99.60 %	
6.500	3.78	0.06 %	0.20 %	0.01 %	99.74 %	
7.000	3.86	0.02 %	0.20 %	0.00 %	99.78 %	
7.400	3.88	0.01 %	0.20 %	0.00 %	99.79 %	
8.000	3.89	0.00 %	0.20 %	0.00 %	99.80 %	
9.000	3.89	0.00 %	0.20 %	0.00 %	99.80 %	
10.000	3.90	0.00 %	0.20 %	0.00 %	99.80 %	
11.000	3.90	0.00 %	0.20 %	0.00 %	99.80 %	
12.000	3.90	0.00 %	0.20 %	0.00 %	99.80 %	

Carbonate and acidity

 Carbonate 0.106 mM
 Acidity error -0.195 mM

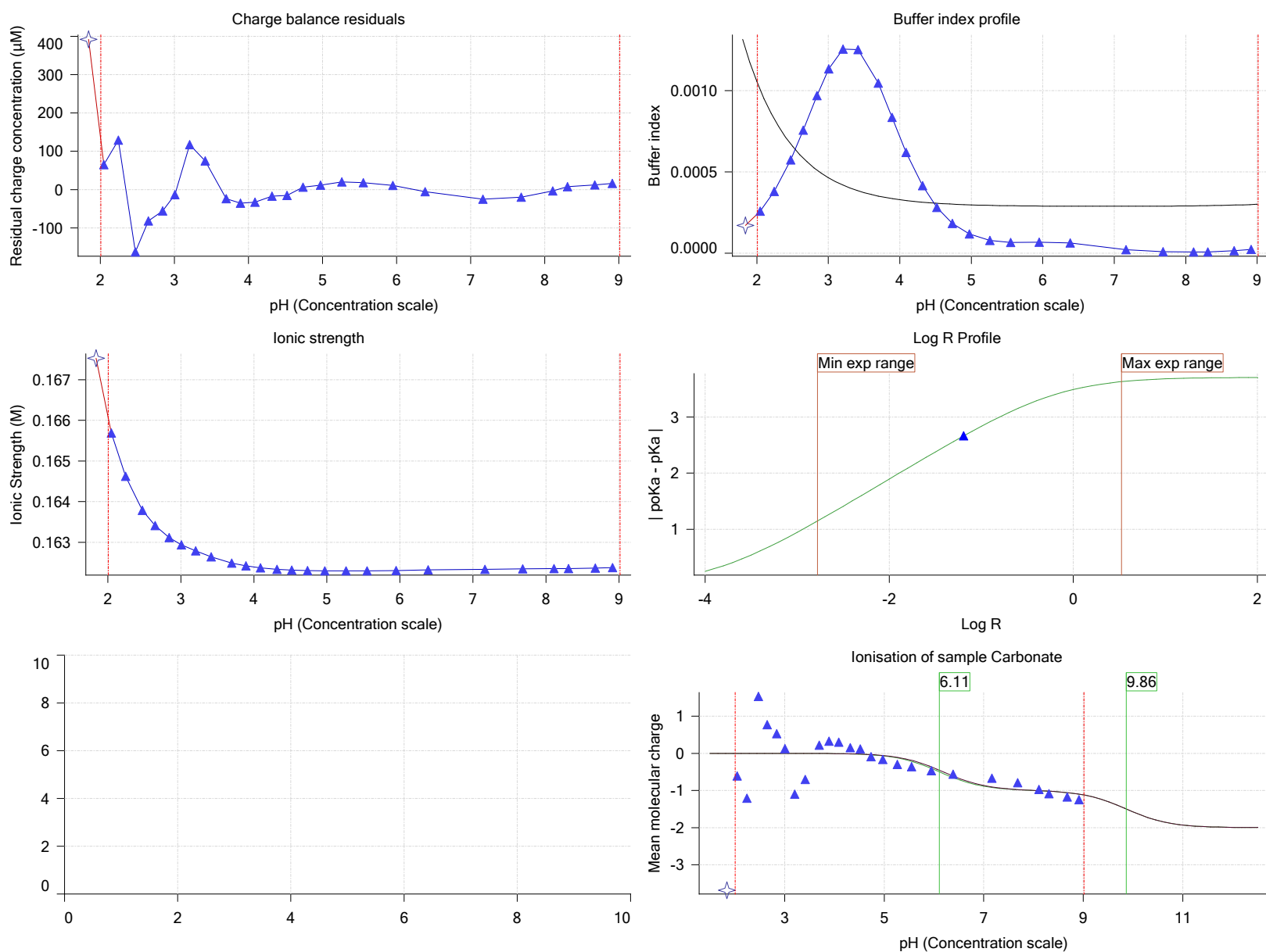
Other graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-24003 Points 53 to 77

Overall results

RMSD 0.260
 Average ionic strength 0.168 M
 Average temperature 24.9°C
 Partition ratio 0.2796 : 1
 Analyte concentration range 1840.5 µM to 1888.2 µM
 Total points considered 23 of 25

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha	0.119	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
S	0.9972	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
jH	0.9	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
jOH	-0.3	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r

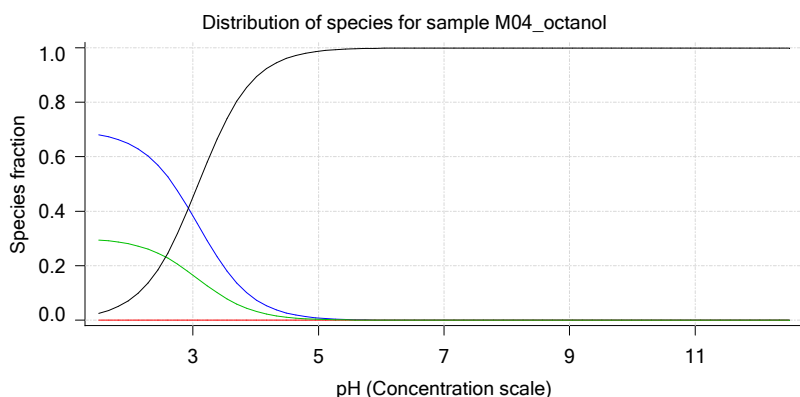
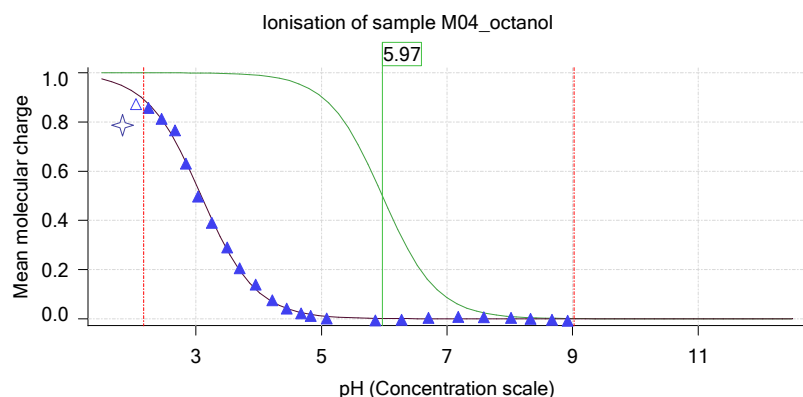
Titrants

0.50 M HCl	0.997124	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
0.50 M KOH	1.003190	3/24/2018 2:50:31 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

M04_octanol concentration factor	0.960
Base pKa 1	5.97
logP (XH +)	0.19
logP (neutral X)	3.59

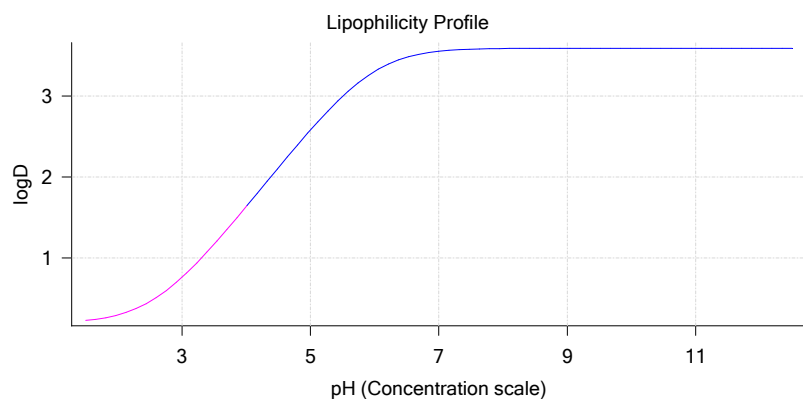
Sample graphs



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 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
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 Instrument ID: **T312060**



Sample graphs (continued)



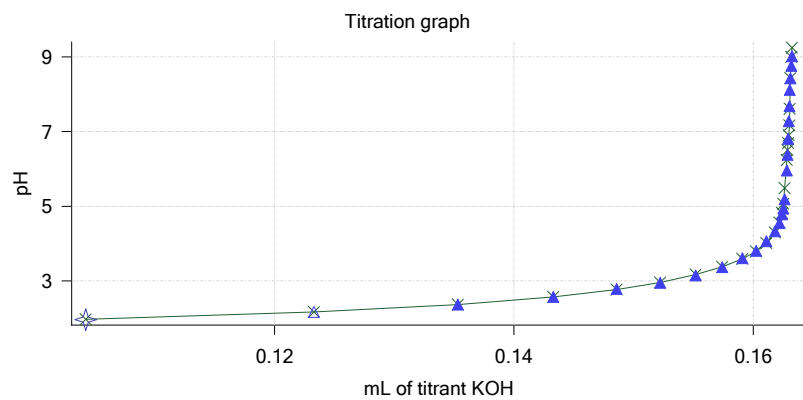
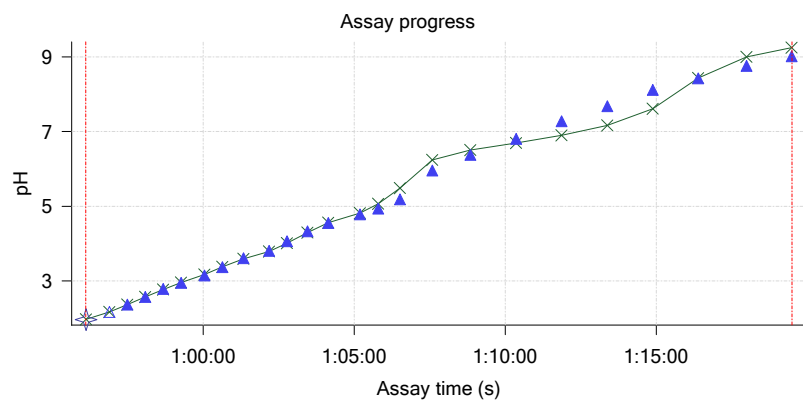
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanolH	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.20	69.22 %	0.00 %	29.97 %	0.81 %	
1.200	0.21	68.89 %	0.00 %	29.83 %	1.28 %	Stomach pH
2.000	0.29	64.50 %	0.01 %	27.93 %	7.57 %	
3.000	0.76	38.35 %	0.04 %	16.61 %	45.00 %	
4.000	1.63	7.59 %	0.08 %	3.29 %	89.04 %	
5.000	2.58	0.84 %	0.09 %	0.36 %	98.70 %	
6.000	3.31	0.09 %	0.09 %	0.04 %	99.79 %	
6.500	3.48	0.03 %	0.09 %	0.01 %	99.87 %	
7.000	3.55	0.01 %	0.09 %	0.00 %	99.90 %	
7.400	3.58	0.00 %	0.09 %	0.00 %	99.90 %	Blood pH
8.000	3.59	0.00 %	0.09 %	0.00 %	99.91 %	
9.000	3.59	0.00 %	0.09 %	0.00 %	99.91 %	
10.000	3.59	0.00 %	0.09 %	0.00 %	99.91 %	
11.000	3.59	0.00 %	0.09 %	0.00 %	99.91 %	
12.000	3.59	0.00 %	0.09 %	0.00 %	99.91 %	

Carbonate and acidity

 Carbonate 0.119 mM
 Acidity error 0.082 mM

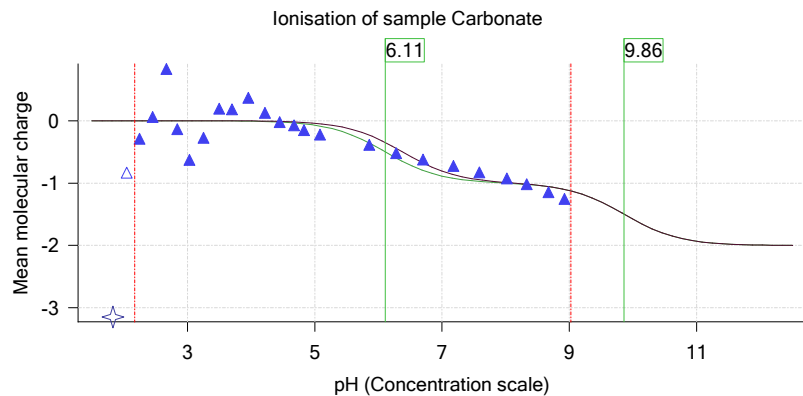
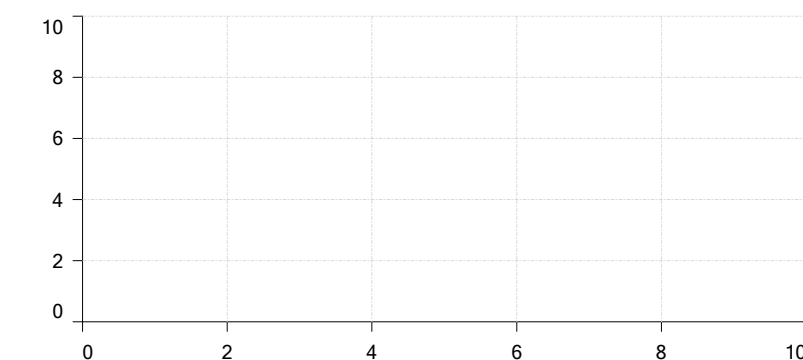
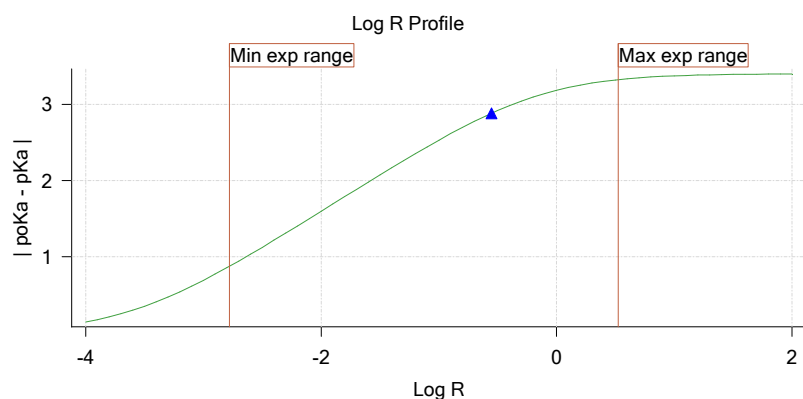
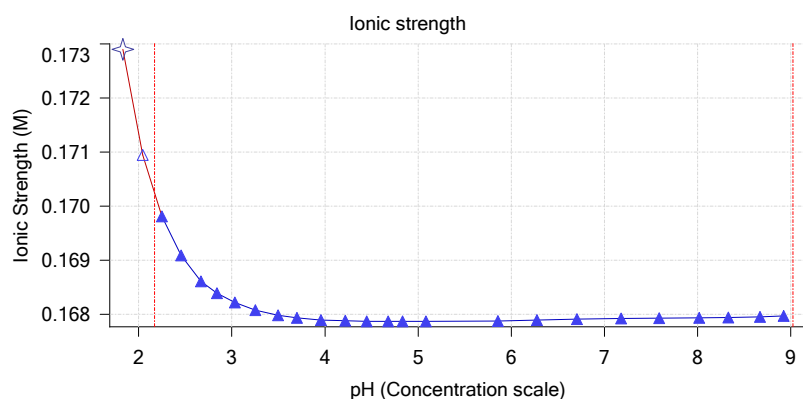
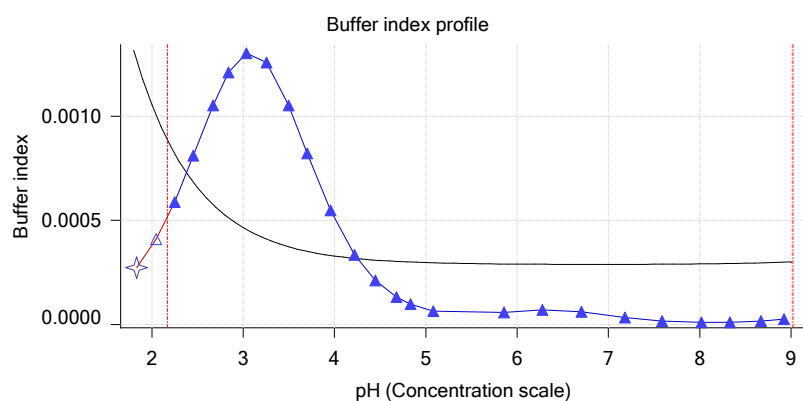
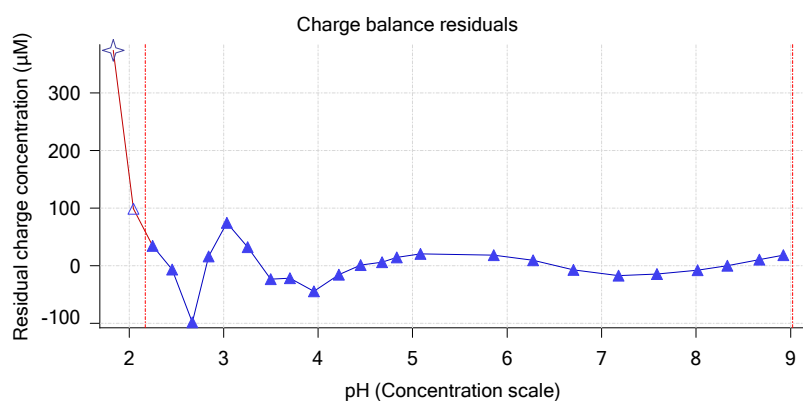
Other graphs



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 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M04_octanol	3/9/2018 4:34:21 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001160 g	3/23/2018 5:00:38 PM	User entered value
Formula weight	269.73 g/mol	3/9/2018 4:34:21 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	269.73	3/9/2018 4:34:21 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	3/9/2018 4:34:21 PM	User entered value
Sample is a	Base	3/9/2018 4:34:21 PM	User entered value
pKa 1	5.97	3/9/2018 4:34:21 PM	User entered value
logp (XH +)	0.19	3/9/2018 4:34:33 PM	User entered value
logP (neutral X)	3.50	3/23/2018 2:32:46 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
4:59.5	Initial pH = 5.97									
8:04.2	Data point 1	1.50000 mL	0.04965 mL	0.00151 mL	0.03001 mL	2.007	0.00427	0.35010	0.00036	10.0 s
8:50.5	Data point 2	1.50000 mL	0.04965 mL	0.01651 mL	0.03001 mL	2.218	-0.00672	0.12678	0.00093	10.0 s
9:26.1	Data point 3	1.50000 mL	0.04965 mL	0.02571 mL	0.03001 mL	2.420	0.00425	0.38859	0.00034	10.0 s
10:01.6	Data point 4	1.50000 mL	0.04965 mL	0.03151 mL	0.03001 mL	2.606	-0.00797	0.19529	0.00089	10.0 s
10:37.2	Data point 5	1.50000 mL	0.04965 mL	0.03532 mL	0.03001 mL	2.816	-0.00186	0.44711	0.00014	10.0 s
11:12.6	Data point 6	1.50000 mL	0.04965 mL	0.03775 mL	0.03001 mL	3.003	0.00280	0.09562	0.00045	10.0 s
11:48.1	Data point 7	1.50000 mL	0.04965 mL	0.03944 mL	0.03001 mL	3.158	0.00375	0.14586	0.00048	10.0 s
12:39.0	Data point 8	1.50000 mL	0.04965 mL	0.04116 mL	0.03001 mL	3.347	-0.00347	0.70036	0.00020	10.0 s
13:24.7	Data point 9	1.50000 mL	0.04965 mL	0.04240 mL	0.03001 mL	3.533	-0.00887	0.63978	0.00055	10.0 s
14:00.2	Data point 10	1.50000 mL	0.04965 mL	0.04341 mL	0.03001 mL	3.695	-0.00873	0.74697	0.00050	10.0 s
14:46.0	Data point 11	1.50000 mL	0.04965 mL	0.04445 mL	0.03001 mL	3.867	-0.01180	0.86864	0.00063	10.0 s
15:21.3	Data point 12	1.50000 mL	0.04965 mL	0.04551 mL	0.03001 mL	4.056	-0.01653	0.82606	0.00090	10.0 s
15:56.8	Data point 13	1.50000 mL	0.04965 mL	0.04659 mL	0.03001 mL	4.268	-0.01706	0.91582	0.00088	10.5 s
16:32.8	Data point 14	1.50000 mL	0.04965 mL	0.04765 mL	0.03001 mL	4.537	-0.01779	0.85452	0.00095	11.5 s
17:14.9	Data point 15	1.50000 mL	0.04965 mL	0.04828 mL	0.03001 mL	4.714	-0.01769	0.95197	0.00089	13.0 s
17:53.3	Data point 16	1.50000 mL	0.04965 mL	0.04866 mL	0.03001 mL	4.876	-0.01700	0.83581	0.00092	13.0 s
18:31.7	Data point 17	1.50000 mL	0.04965 mL	0.04897 mL	0.03001 mL	5.040	-0.01747	0.89358	0.00091	14.0 s
19:11.1	Data point 18	1.50000 mL	0.04965 mL	0.04920 mL	0.03001 mL	5.236	-0.01840	0.90934	0.00095	15.5 s
20:02.3	Data point 19	1.50000 mL	0.04965 mL	0.04944 mL	0.03001 mL	5.461	-0.01934	0.94812	0.00098	21.5 s
20:54.3	Data point 20	1.50000 mL	0.04965 mL	0.04965 mL	0.03001 mL	5.969	-0.01829	0.93298	0.00093	36.0 s
21:55.7	Data point 21	1.50000 mL	0.04965 mL	0.04974 mL	0.03001 mL	6.338	-0.01998	0.98727	0.00099	53.0 s
23:19.4	Data point 22	1.50000 mL	0.04965 mL	0.04981 mL	0.03001 mL	6.965	-0.05661	0.98918	0.00281	Timed out at 59.5 s
24:55.0	Data point 23	1.50000 mL	0.04965 mL	0.04988 mL	0.03001 mL	7.732	-0.10014	0.99537	0.00496	Timed out at 59.5 s
26:25.5	Data point 24	1.50000 mL	0.04965 mL	0.04993 mL	0.03001 mL	8.300	-0.05511	0.99507	0.00273	Timed out at 59.5 s
28:01.1	Data point 25	1.50000 mL	0.04965 mL	0.05000 mL	0.03001 mL	8.709	-0.01976	0.97372	0.00099	56.5 s
29:33.2	Data point 26	1.50000 mL	0.04965 mL	0.05007 mL	0.03001 mL	9.016	-0.01909	0.93060	0.00098	43.0 s
31:16.2	Data point 27	1.50000 mL	0.10503 mL	0.05007 mL	0.11002 mL	1.966	-0.00262	0.17546	0.00031	10.0 s
32:02.5	Data point 28	1.50000 mL	0.10503 mL	0.06689 mL	0.11002 mL	2.167	-0.00002	0.00005	0.00013	10.0 s
32:38.3	Data point 29	1.50000 mL	0.10503 mL	0.07808 mL	0.11002 mL	2.360	-0.00053	0.02080	0.00018	10.0 s
33:13.7	Data point 30	1.50000 mL	0.10503 mL	0.08530 mL	0.11002 mL	2.588	0.00069	0.01014	0.00034	10.0 s
33:49.3	Data point 31	1.50000 mL	0.10503 mL	0.08972 mL	0.11002 mL	2.762	-0.00184	0.09470	0.00030	10.0 s
34:35.2	Data point 32	1.50000 mL	0.10503 mL	0.09306 mL	0.11002 mL	2.952	-0.00238	0.48804	0.00017	10.5 s
35:11.1	Data point 33	1.50000 mL	0.10503 mL	0.09534 mL	0.11002 mL	3.117	-0.00618	0.30787	0.00055	10.0 s
36:02.2	Data point 34	1.50000 mL	0.10503 mL	0.09781 mL	0.11002 mL	3.314	-0.00705	0.70654	0.00041	10.0 s
36:53.1	Data point 35	1.50000 mL	0.10503 mL	0.09939 mL	0.11002 mL	3.524	-0.00556	0.85447	0.00030	10.0 s
37:28.6	Data point 36	1.50000 mL	0.10503 mL	0.10080 mL	0.11002 mL	3.806	-0.00526	0.75008	0.00030	10.0 s
38:09.2	Data point 37	1.50000 mL	0.10503 mL	0.10162 mL	0.11002 mL	3.999	-0.01309	0.90328	0.00068	10.0 s



Assay Events

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24003**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
38:49.7	Data point 38	1.50000 mL	0.10503 mL	0.10228 mL	0.11002 mL	4.196	-0.00633	0.53369	0.00043	10.0 s
39:35.4	Data point 39	1.50000 mL	0.10503 mL	0.10285 mL	0.11002 mL	4.425	-0.01381	0.73265	0.00080	10.0 s
40:10.8	Data point 40	1.50000 mL	0.10503 mL	0.10315 mL	0.11002 mL	4.625	0.00050	0.00129	0.00069	10.5 s
40:57.0	Data point 41	1.50000 mL	0.10503 mL	0.10343 mL	0.11002 mL	4.842	-0.01579	0.77724	0.00088	11.0 s
41:38.5	Data point 42	1.50000 mL	0.10503 mL	0.10360 mL	0.11002 mL	5.078	-0.00838	0.38707	0.00067	11.5 s
42:25.7	Data point 43	1.50000 mL	0.10503 mL	0.10374 mL	0.11002 mL	5.365	-0.00881	0.23766	0.00089	12.0 s
43:08.2	Data point 44	1.50000 mL	0.10503 mL	0.10381 mL	0.11002 mL	5.655	-0.01757	0.85957	0.00094	13.5 s
43:52.2	Data point 45	1.50000 mL	0.10503 mL	0.10388 mL	0.11002 mL	6.051	-0.01851	0.93922	0.00094	41.5 s
45:04.4	Data point 46	1.50000 mL	0.10503 mL	0.10393 mL	0.11002 mL	6.487	-0.02808	0.98839	0.00139	Timed out at 59.5 s
46:29.9	Data point 47	1.50000 mL	0.10503 mL	0.10398 mL	0.11002 mL	7.265	-0.09351	0.99809	0.00462	Timed out at 59.5 s
48:00.3	Data point 48	1.50000 mL	0.10503 mL	0.10402 mL	0.11002 mL	7.780	-0.09755	0.99711	0.00483	Timed out at 59.5 s
49:35.9	Data point 49	1.50000 mL	0.10503 mL	0.10409 mL	0.11002 mL	8.206	-0.05783	0.98965	0.00287	Timed out at 59.5 s
51:06.4	Data point 50	1.50000 mL	0.10503 mL	0.10414 mL	0.11002 mL	8.404	-0.03670	0.98260	0.00183	Timed out at 59.5 s
52:36.9	Data point 51	1.50000 mL	0.10503 mL	0.10419 mL	0.11002 mL	8.772	-0.02623	0.91998	0.00135	Timed out at 59.5 s
54:07.4	Data point 52	1.50000 mL	0.10503 mL	0.10423 mL	0.11002 mL	9.008	-0.01967	0.95537	0.00099	37.0 s
56:07.6	Data point 53	1.50000 mL	0.16334 mL	0.10423 mL	0.51002 mL	1.958	-0.00498	0.69174	0.00030	10.0 s
56:53.8	Data point 54	1.50000 mL	0.16334 mL	0.12331 mL	0.51002 mL	2.165	0.01137	0.42530	0.00086	10.0 s
57:29.6	Data point 55	1.50000 mL	0.16334 mL	0.13533 mL	0.51002 mL	2.365	-0.01105	0.37291	0.00089	10.0 s
58:05.2	Data point 56	1.50000 mL	0.16334 mL	0.14330 mL	0.51002 mL	2.569	-0.00999	0.57469	0.00065	10.0 s
58:40.8	Data point 57	1.50000 mL	0.16334 mL	0.14859 mL	0.51002 mL	2.782	-0.00724	0.84718	0.00039	10.0 s
59:16.3	Data point 58	1.50000 mL	0.16334 mL	0.15221 mL	0.51002 mL	2.951	-0.00453	0.17701	0.00053	10.5 s
1:00:02.6	Data point 59	1.50000 mL	0.16334 mL	0.15520 mL	0.51002 mL	3.145	-0.00569	0.12433	0.00080	10.0 s
1:00:38.1	Data point 60	1.50000 mL	0.16334 mL	0.15741 mL	0.51002 mL	3.364	-0.01891	0.93813	0.00096	16.5 s
1:01:20.1	Data point 61	1.50000 mL	0.16334 mL	0.15910 mL	0.51002 mL	3.607	-0.00838	0.90591	0.00043	10.0 s
1:02:11.1	Data point 62	1.50000 mL	0.16334 mL	0.16023 mL	0.51002 mL	3.809	-0.01009	0.62944	0.00063	10.0 s
1:02:46.4	Data point 63	1.50000 mL	0.16334 mL	0.16110 mL	0.51002 mL	4.063	-0.01406	0.72392	0.00082	10.0 s
1:03:27.2	Data point 64	1.50000 mL	0.16334 mL	0.16181 mL	0.51002 mL	4.326	-0.01356	0.90136	0.00070	10.5 s
1:04:08.2	Data point 65	1.50000 mL	0.16334 mL	0.16218 mL	0.51002 mL	4.555	-0.01747	0.81566	0.00096	37.5 s
1:05:11.2	Data point 66	1.50000 mL	0.16334 mL	0.16239 mL	0.51002 mL	4.783	-0.01567	0.79185	0.00087	11.0 s
1:05:47.6	Data point 67	1.50000 mL	0.16334 mL	0.16251 mL	0.51002 mL	4.937	-0.01579	0.62099	0.00099	12.5 s
1:06:30.6	Data point 68	1.50000 mL	0.16334 mL	0.16263 mL	0.51002 mL	5.187	-0.01710	0.86918	0.00091	34.0 s
1:07:35.2	Data point 69	1.50000 mL	0.16334 mL	0.16279 mL	0.51002 mL	5.960	-0.01912	0.94697	0.00097	45.0 s
1:08:50.9	Data point 70	1.50000 mL	0.16334 mL	0.16287 mL	0.51002 mL	6.378	-0.03153	0.95619	0.00159	Timed out at 59.5 s
1:10:21.3	Data point 71	1.50000 mL	0.16334 mL	0.16291 mL	0.51002 mL	6.803	-0.06207	0.98528	0.00309	Timed out at 59.5 s
1:11:51.8	Data point 72	1.50000 mL	0.16334 mL	0.16296 mL	0.51002 mL	7.279	-0.09237	0.99346	0.00458	Timed out at 59.5 s
1:13:22.3	Data point 73	1.50000 mL	0.16334 mL	0.16301 mL	0.51002 mL	7.684	-0.09598	0.99125	0.00476	Timed out at 59.5 s
1:14:52.8	Data point 74	1.50000 mL	0.16334 mL	0.16305 mL	0.51002 mL	8.114	-0.08212	0.99372	0.00407	Timed out at 59.5 s
1:16:23.3	Data point 75	1.50000 mL	0.16334 mL	0.16310 mL	0.51002 mL	8.426	-0.04721	0.97560	0.00236	Timed out at 59.5 s
1:17:58.8	Data point 76	1.50000 mL	0.16334 mL	0.16317 mL	0.51002 mL	8.764	-0.01810	0.93699	0.00092	59.0 s
1:19:28.4	Data point 77	1.50000 mL	0.16334 mL	0.16324 mL	0.51002 mL	9.016	-0.00920	0.71690	0.00054	30.0 s
1:20:07.6	Assay volumes	1.50000 mL	0.16334 mL	0.16324 mL	0.51002 mL					

Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.030 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.080 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24003**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.400 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.119	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus S	0.9972	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus jH	0.9	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus jOH	-0.3	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r
Base concentration factor	1.003	3/24/2018 2:50:31 AM	C:\Sirius_T3\KOH18C23.t3r
Acid concentration factor	0.997	3/24/2018 2:50:31 AM	C:\Sirius_T3\HCl18C23.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	3/16/2018 11:09:18 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	03-16-2018	3/16/2018 10:56:23 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3/22/2018	3/23/2018 9:34:17 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24003**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 2:50:31 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titration		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+5.05 mV		3/24/2018 2:50:59 AM
Filling solution	3M KCl	KCL097	3/23/2018 9:29:07 AM
Liquids			
Wash 1	50% IPA:50% Water		3/23/2018 9:29:12 AM
Wash 2	0.5% Triton X-100 in H2O		3/23/2018 9:29:15 AM
Buffer position 1	pH7 Wash		3/23/2018 9:29:19 AM
Buffer position 2	pH 7		3/23/2018 9:29:21 AM
Storage position			3/23/2018 9:30:23 AM
Wash water	7.6e+003 mL	03-12-2018	3/12/2018 9:25:04 AM
Waste	2.6e+003 mL		3/12/2018 9:24:49 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	162:53:01		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		



Assay Settings

Sample name: **M04_octanol** Experiment start time: **3/24/2018 2:50:31 AM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-24003** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24003_M04_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00